Virtual Design and Optimization of Metallic Glass Alloys

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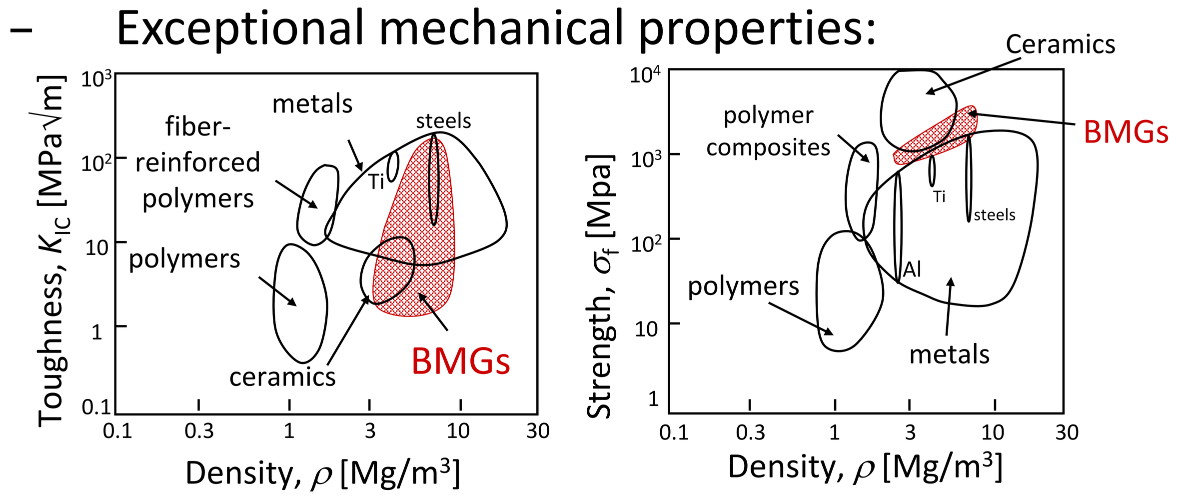
Goal

Develop the tools necessary to virtually optimize a metallic glass alloy for several properties

Background

Metallic Glasses: Metals without crystalline order

- Exceptional mechanical properties:



- Easy to form: Can be shaped like plastics
- Current and promising applications:
  - Hard-tissue implants
  - Casings for electronics

Advanced Materials 22 (2010): 1566-597.

Key limitations:

1. Not all alloys can form in glassy state
2. Lack of methodology to design properties

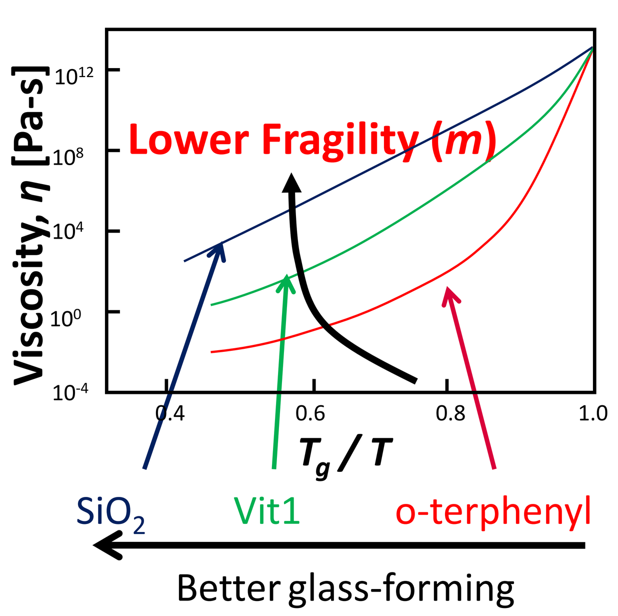
Calculating Glass-Forming Ability

Background: What are good measurements?

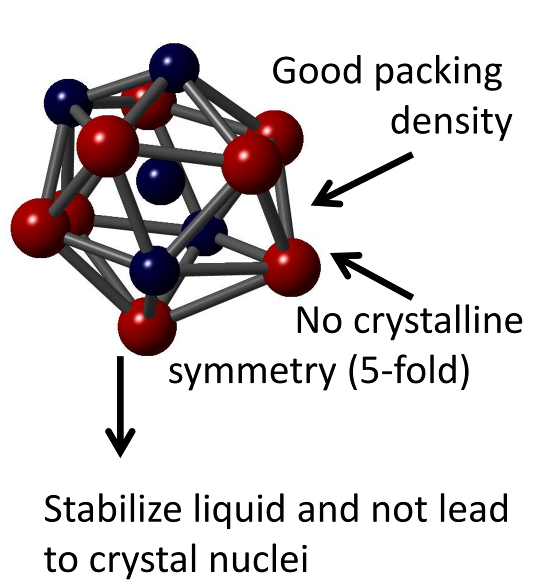
- Direct measure: Critical cooling rate
  - Slowest rate that bypasses crystallization
  - Calculation time: 200 years on 20 CPUs
- Proposed method: *Kinetics* and *driving force*

Calculation strategy: Computational feasibility

	Kinetics	*Driving Force*
Behavior:	High Viscosity	Stable clusters
Rationale:	Slow diffusion	Low free energy
Parameter:	Fragility	Icosahedron Fraction



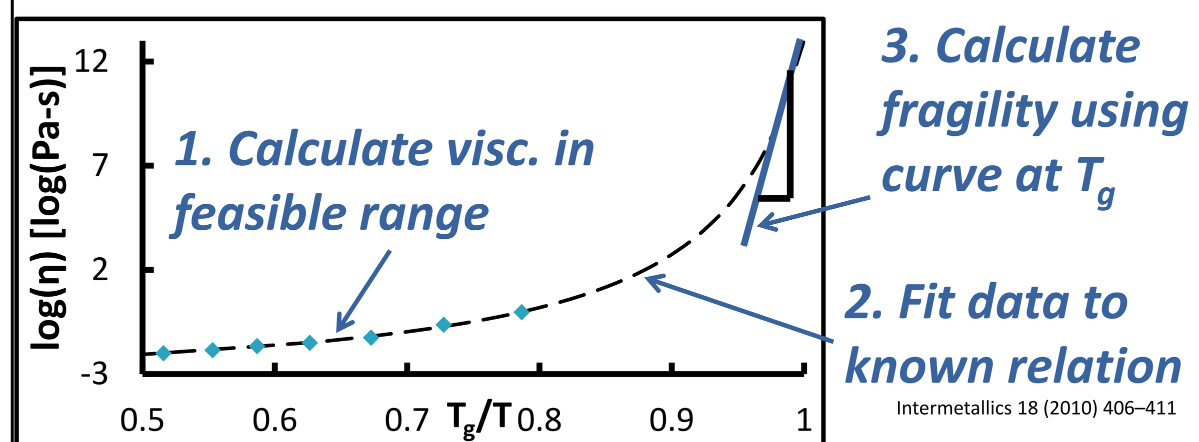
Adapted from: Mat. Sci. and Eng. R. 45-89 (2004).



Physical Review B. 72 (2005) 174107

Calculation Strategy

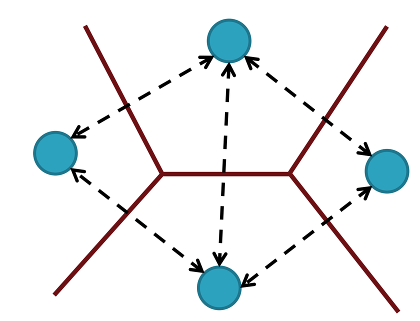
Fragility: Change in liquid viscosity



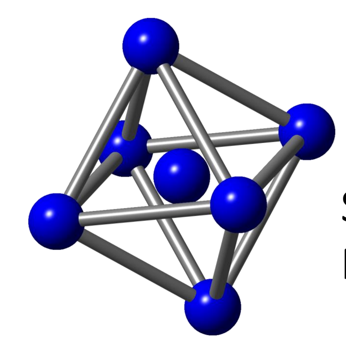
Intermetallics 18 (2010) 406–411

Icosahedron Fraction: Local order analysis

1. Identify neighbors: Voronoi analysis



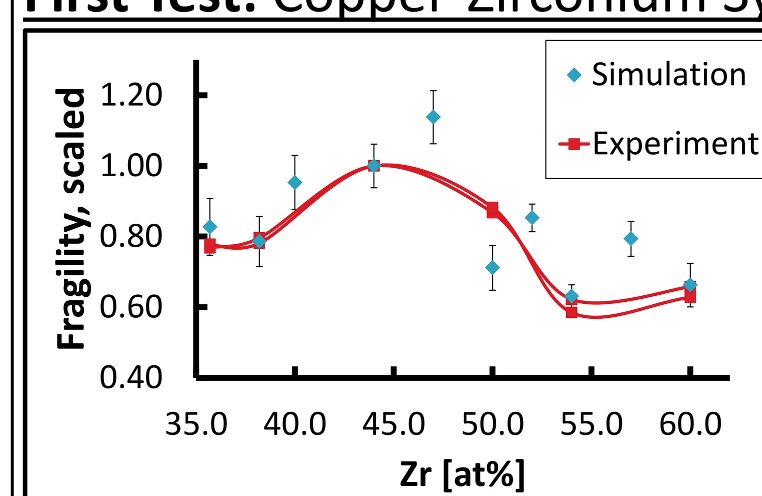
2. Identify polyhedra: Connectivity of neighbors



Six neighbors: Four bonds each

Glass-Forming Ability Results

First Test: Copper-Zirconium System



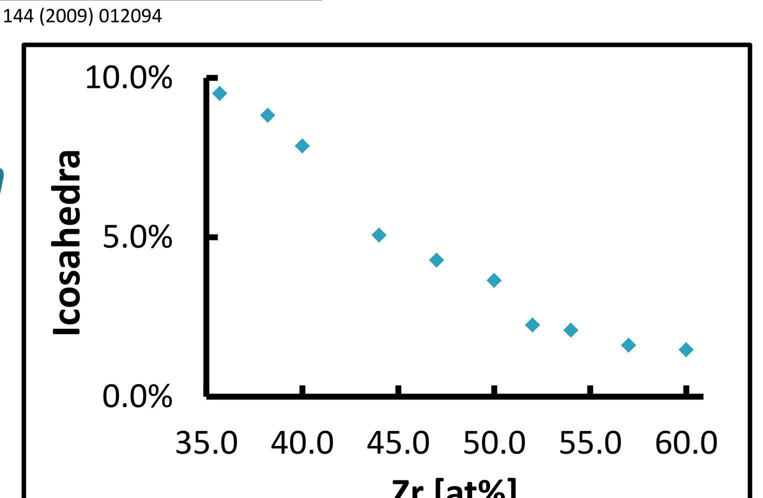
Data from: Journal of Physics: Conference Series 144 (2009) 012094

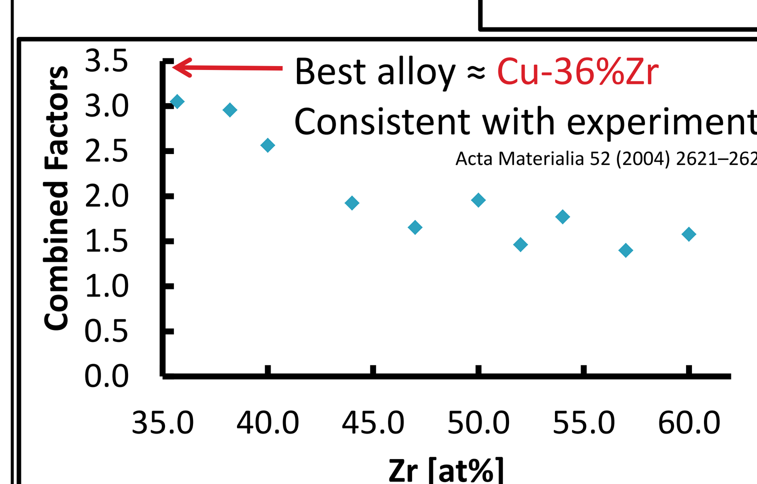
1. Derive fragility from calculated viscosity profile

Two regions of slow dynamics

2. Find system icosahedra fraction

More stability with greater copper fraction





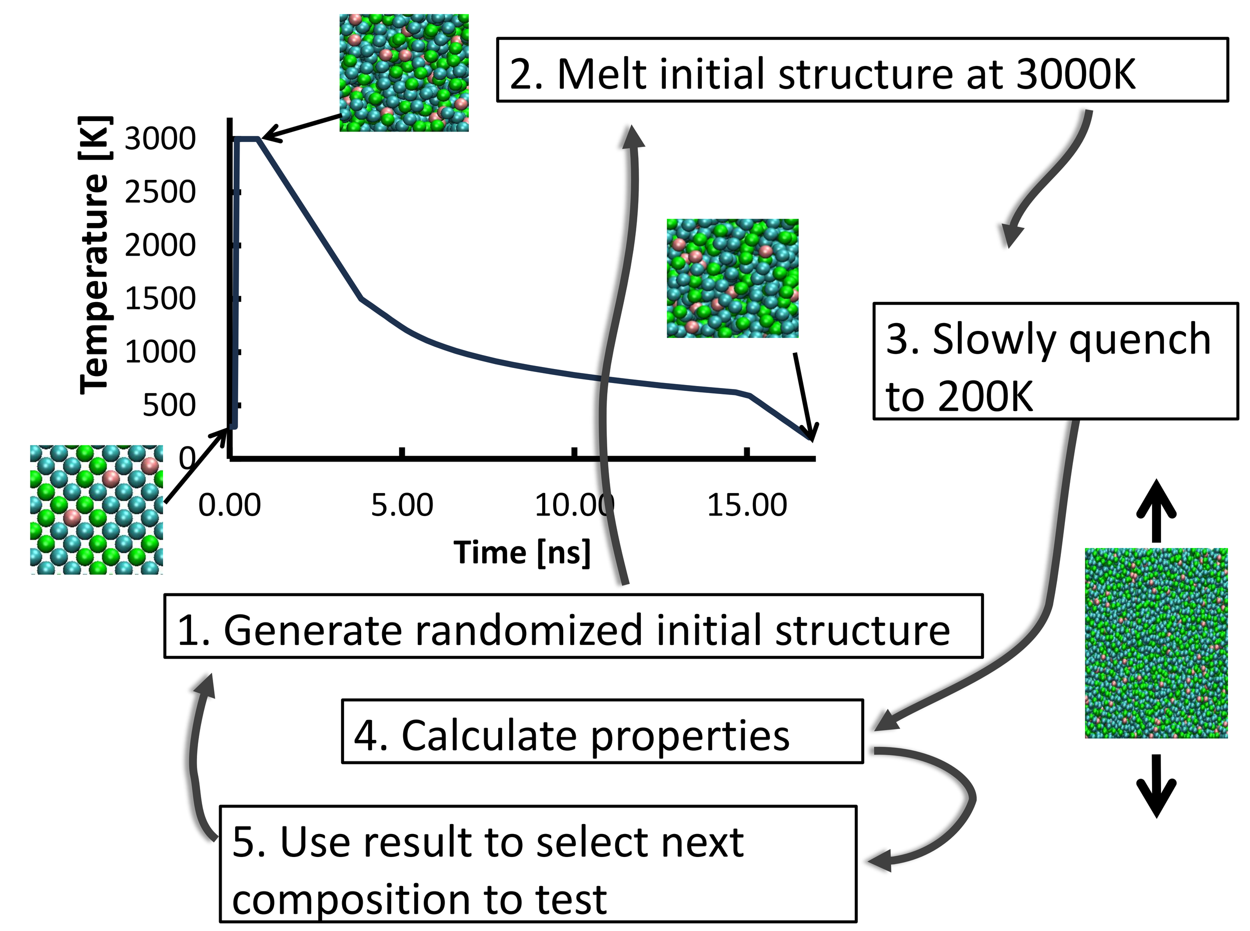
3. Combine the two effects

Used simple relation:

$$V = \frac{\overline{m}}{m} + \frac{Icos}{\overline{Icos}}$$

Discussion of Results

- Selected alloy matches experimental results
- Methods can be applied to new system



Design Criteria

Target System:	Ternary Metallic Glasses
Available Components:	Cu, Ag, Ni, Zr, Ti, Al
Material Properties:	$A_xB_yC_{100-(x+y)}$

1. Material Cost
2. Density
3. Elastic Modulus
4. Fracture Toughness
5. Yield Strength

Composition:	Solute <90%, 0.2% spacing
Possible combinations:	Over *2 million*
Additional Constraint:	**Alloy can form in glassy state**

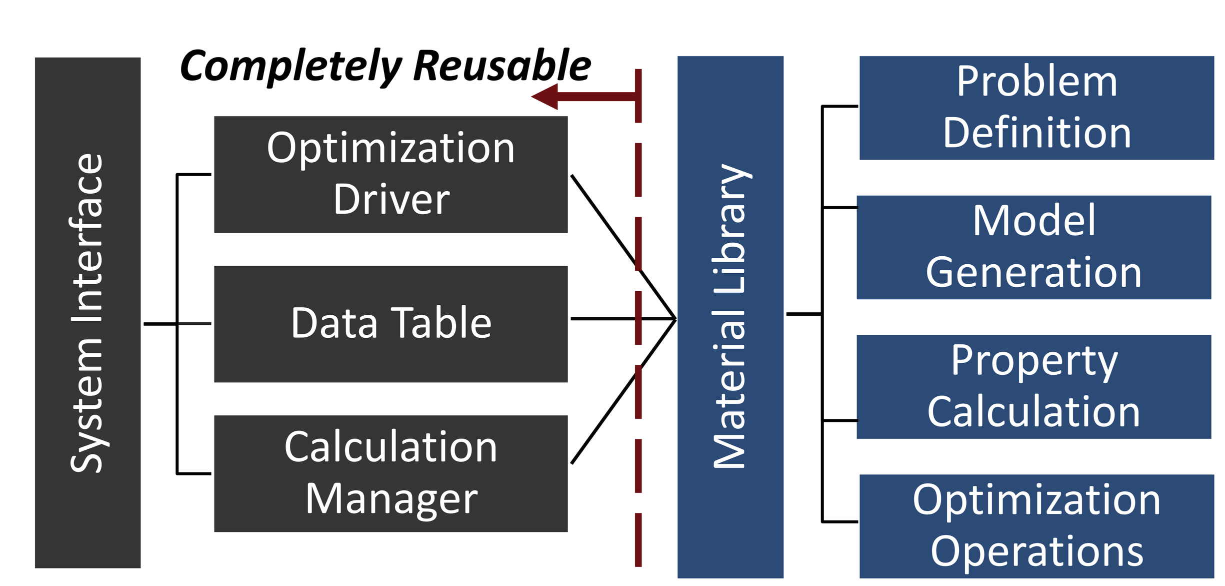
Optimization Technique

Method Selection: Genetic Algorithms

- Successfully used in previous work
- Several key advantages:
  - Can find a global maximum
  - Does not require derivatives

Calculation Management System

- Developed and implemented design program
  - Manages selection and property calculation
- Designed to allow for easy adaptation
  - Of the 3600 lines, at least 3100 reusable



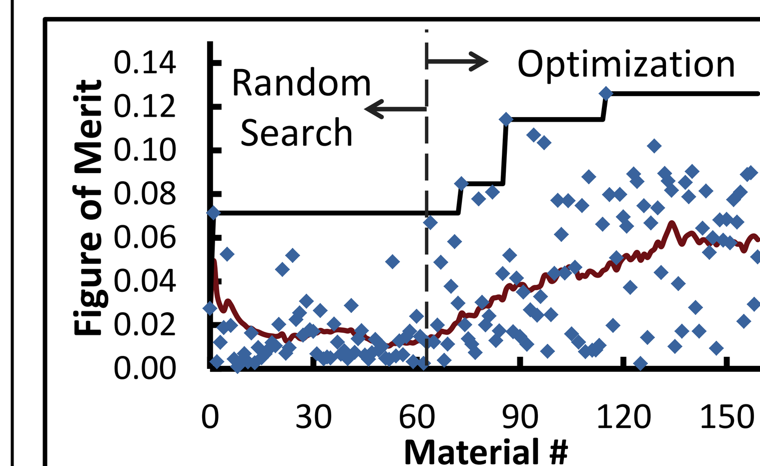
Property Optimization

Initial Test of Design Software

Figure of merit: $\frac{[Fracture\ Toughness]}{[Elastic\ Modulus][Density]}$

Results of Calculations

Run Time:	3 weeks
Processor Usage:	3.5 CPU years



Large increase in figure of merit with genetic algorithm

Sample Alloy Selection

Best Compositions	*Figure of Merit*
1. Al-19.2at%Ag-5.8at%Zr	0.126
2. Al-25.0at%Ni-8.6at%Zr	0.114
3. Al-19.0at%Ag-7.4at%Zr	0.107

Recommended Alloy: Al-19%Ag-6%Zr

Discussion of recommendation:

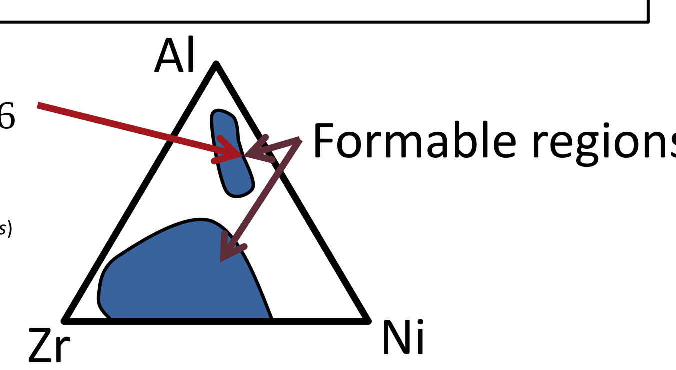
- No known Al-Ag-Zr metallic glasses
- Al-Ni-Zr: Known for ductile glasses

J. Of Material Science Letters. 7 (1988) 805-807

$Al_{66.4}Ni_{25}Zr_{8.6}$

Formable by melt-spinning

(Source: Phase Diagrams and Physical Properties of Equilibrium Alloys)



Conclusions

Glass-Forming Ability Calculation

- Identified best glass-forming Cu-Zr alloy
- Kinetics and driving force method found suitable

Property Optimization

- Property optimization yields results in 3 weeks
- Selected alloys are physically reasonable

Future Work

- Improve accuracy of aluminum potential
- Directly screen for glass-forming
- Integrate with experimental methods

Acknowledgements

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